Lawrence Livermore National Laboratory

Non-LTE Plasma Modeling with Cretin

2011 International Workshop On EUV and Soft X-Ray Sources

Howard Scott

8 November, 2011

Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

A brief history of Cretin

- Started ~1984 as a tool for modeling accretion disk spectra (LTE only)
- Added non-LTE capability in late 1980's
  - Platform for developing non-LTE radiation transport algorithms
  - Applications – X-ray lasers, laser-produced plasmas
  - Atomic kinetics driven by external atomic models
- Fusion applications (inertial & magnetic) important from early 1990's
  - Spectroscopic diagnostics for ICF
  - Energy balance for MFE (impurities + divertor region)
  - More emphasis on line shapes and dense plasma effects
- Development of compact inline atomic models dates from early 2000's
  - Used within radiation-hydrodynamics simulations
  - Allow quick scoping studies
  - Helpful for developing detailed atomic models

All physical processes in Cretin are driven by non-LTE atomic kinetics

- Uses either external atomic data files or internally generated models
- Multiple species handled simultaneously
- Atomic processes included: (+ all inverse processes)
  - radiative excitation, ionization
  - electron-ion, and ion-ion collisional excitation, ionization
  - autoionization / dielectronic recombination
- Maxwellian or (partially) non-thermal electron distributions
- Implicit solution for populations (steady-state or time-dependent)
- Iterated to consistency with all other physical processes
  - radiation transport
  - conduction
  - energy balance / temperature evolution
  - Lagrangian MHD (1D only)
  - laser absorption

Radiation transport in Cretin comes in different flavors

Continuum, lines and spectra are treated separately for efficiency

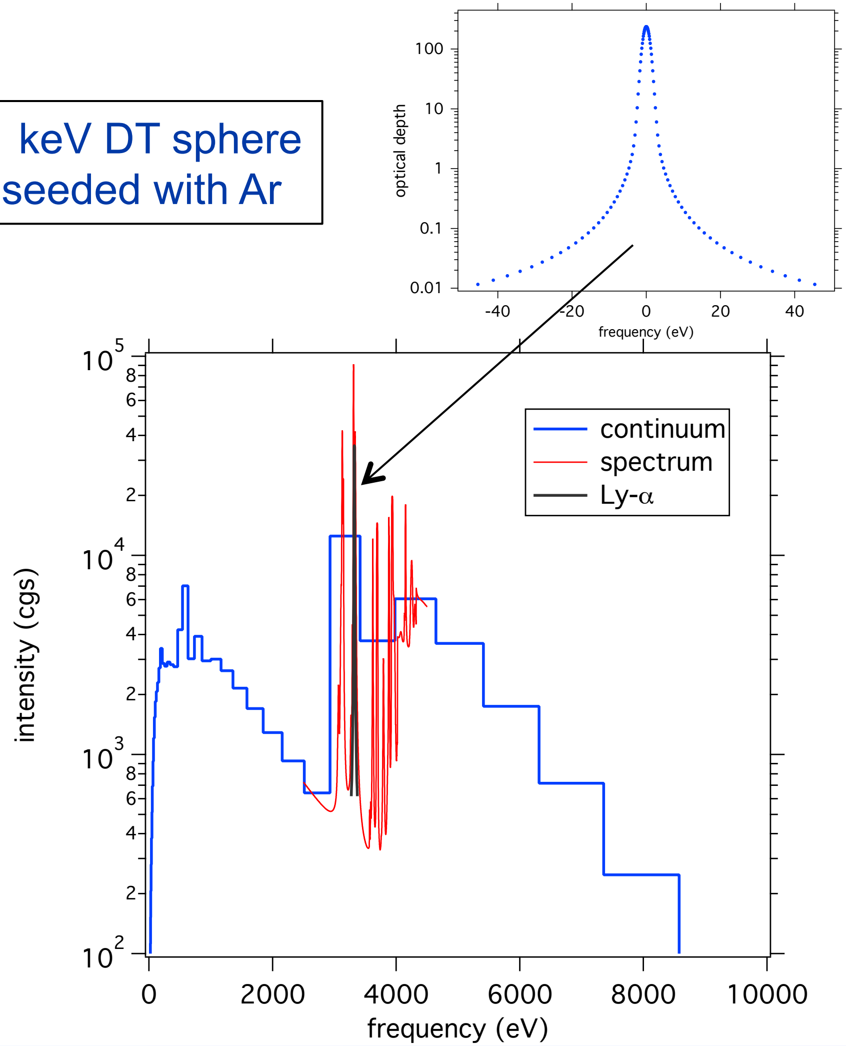
Iterated to consistency with atomic kinetics (and other processes):

- coarsely-binned continuum radiation over full energy range for evaluating photo rates
- finely-binned line radiation for resolving individual line profiles

Evaluated after convergence:

- spectral radiation on fine bins to resolve features in energy range(s) of interest

1 keV DT sphere seeded with Ar



Radiation transport (continued)

- Radiation transport is available in:
  - 1D (planar, cylindrical, spherical) / 2D (xy, rz) / 3D (xyz)
- Uses discrete ordinates methods
  - 1D – long characteristics, 2D / 3D – short characteristics
- Line radiation algorithms handle multiple effects:
  - overlapping / interacting lines
  - Doppler shifting
  - Voigt profiles with complete or partial redistribution

    – or –

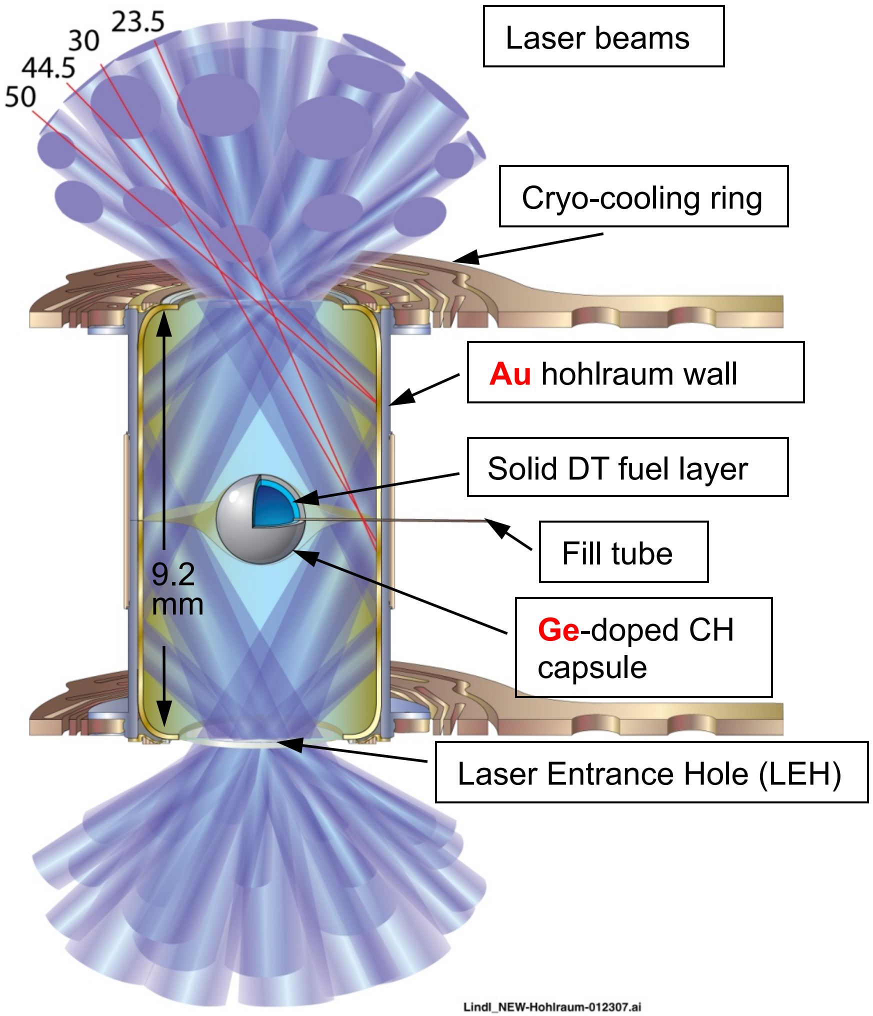
    Stark profiles calculated in-line
- Self-consistency with atomic kinetics achieved through a linearization procedure combined with accelerated lambda iteration
- Escape factors are also available for all geometries and dimensionalities

Compact atomic models

- Requirements:
  - Model any combination of elements (including high Z)
  - Cover a wide range of conditions (near-neutral to fully-stripped)
  - Flexible construction for investigating structure
    e.g. high-N states, inner-shell holes, doubly-, triply-excited states
  - Not “too” expensive
- Current approach:
  - Superconfigurations based on principal quantum numbers
  - Screened-hydrogenic energy levels
  - Simple formulas for transition rates
  - ~20 levels per ionization stage
  - Use of some tabulated data improves accuracy considerably
    - ionization energies, term-split oscillator strengths and energies

H. A. Scott and S. B. Hansen, HEDP 6, 39-47 (2010)

Cretin is used heavily in simulations for the National Ignition Facility (NIF)

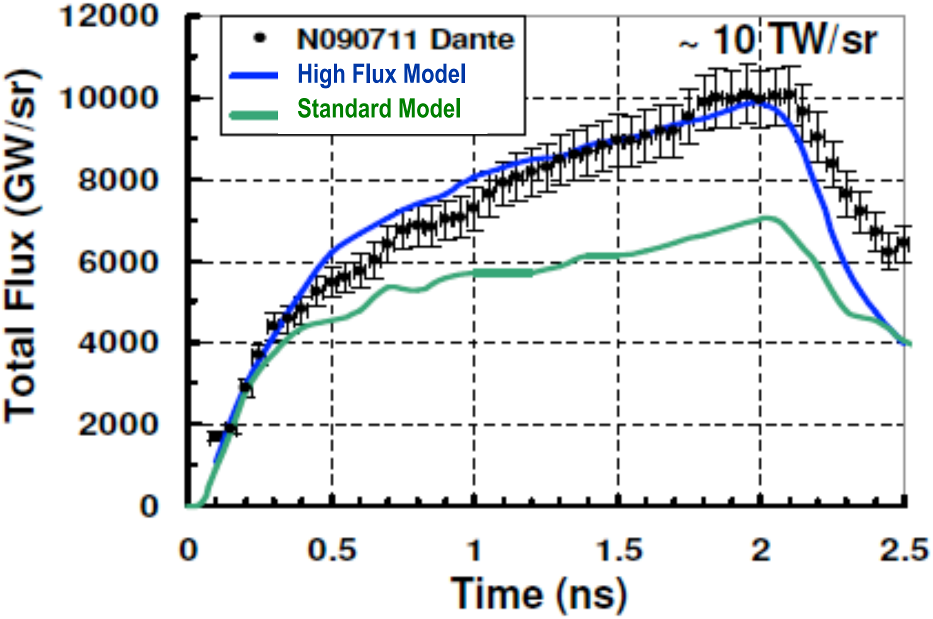


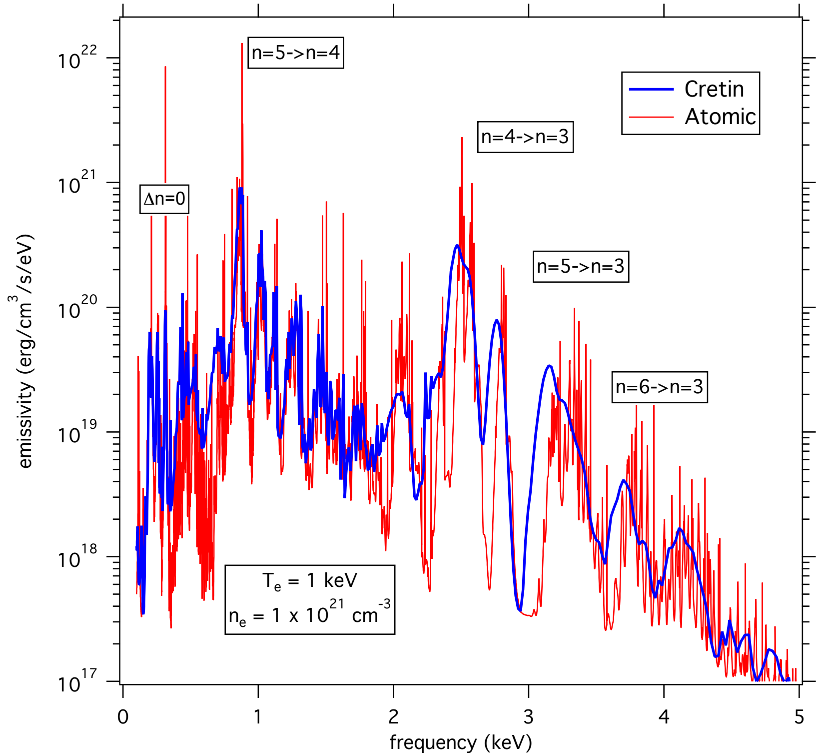
- Au from hohlraum wall converts laser energy to X-rays which drive capsule implosion
  - T_e < 3 keV, $\rho \sim 0.01\text{-}\ 0.1\ \text{g/cm}^3$
- Ge in capsule shields fuel from X-ray preheat
  - T_e < 200 eV, $\rho \sim 0.1\text{-}100\ \text{g/cm}^3$
- Ge in fuel provides spectral signature of instability growth
  - $T_e \sim 2\text{-}3$ keV, $\rho \sim 100\ \text{g/cm}^3$

NLTE physics is integrated into the rad-hydro simulations using the compact atomic models developed in Cretin

The compact models work very well in hohlraum simulations

Vacuum hohlraum
Olsen, et al, IFSA 2009





These models are a critical part of the High Flux Model (HFM)
Rosen, et al, HEDP **7**, 180 (2011)

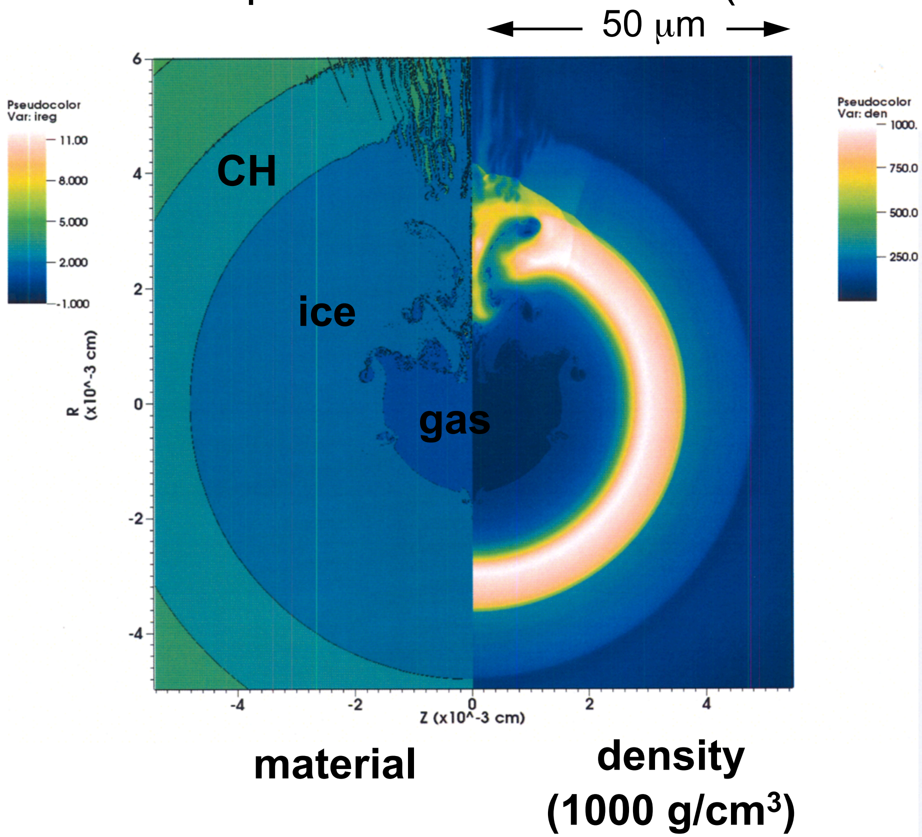
Integrated emission above 1.8 keV differs by ~20%

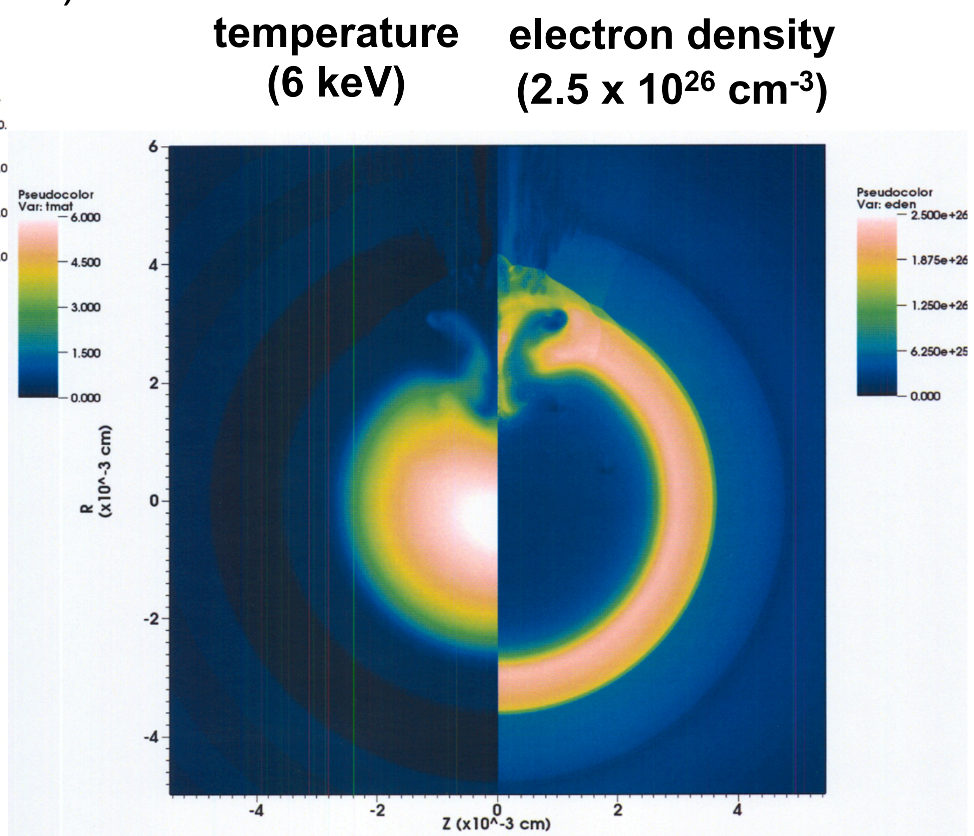
Atomic results provided by C. Fontes

Using Cretin as a postprocessor permits use of more detailed atomic models

- 2D high-resolution HYDRA simulation w/ perturbation due to fill tube
- Postprocessed with Cretin (deresolved)

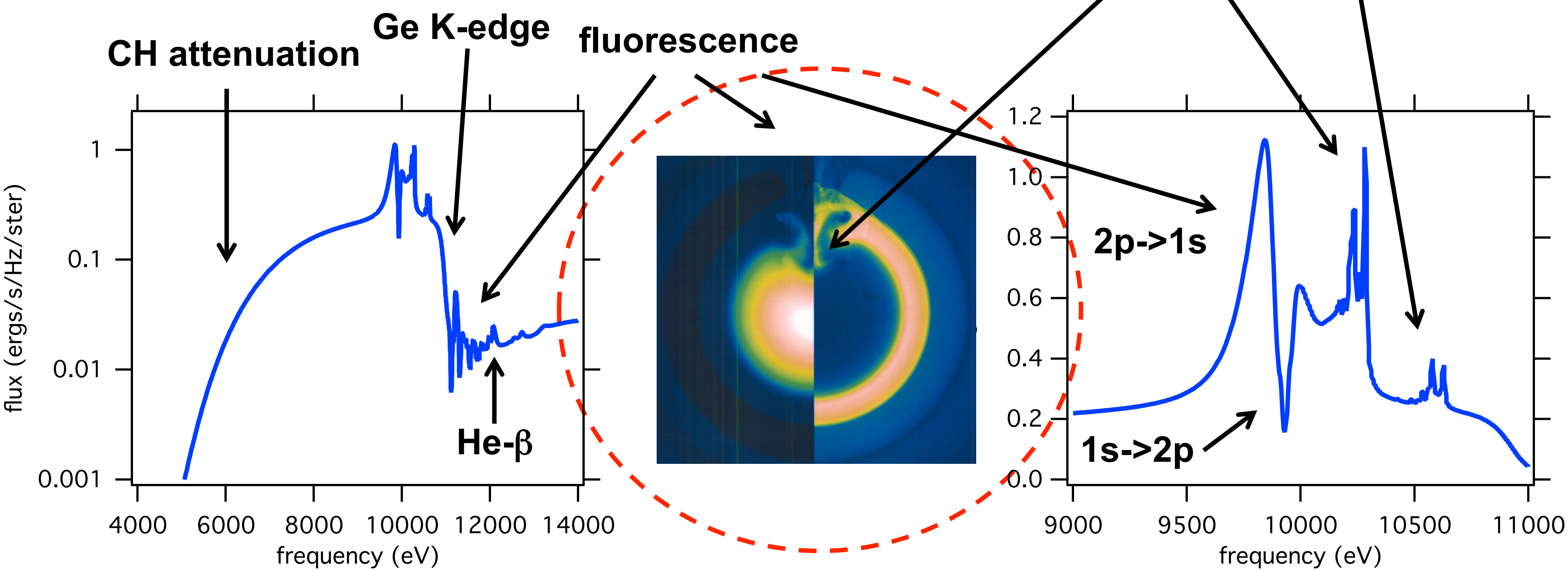
B. A. Hammel, et al, Phys. Plasmas **18**, 056310 (2011)





Combining detailed and compact models provides spectroscopic accuracy with wide coverage

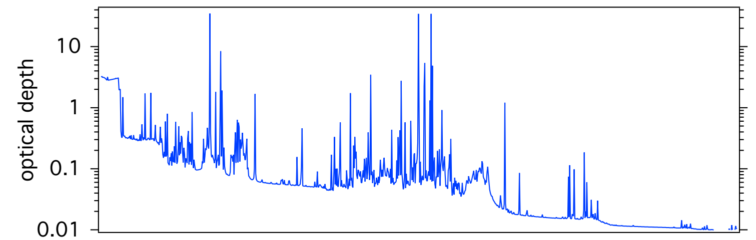
- K-shell emission from hot Ge (>2 keV)
- 1s->2p absorption from warm Ge (300 eV)
- 2p->1s fluorescence from cold Ge (200 eV)

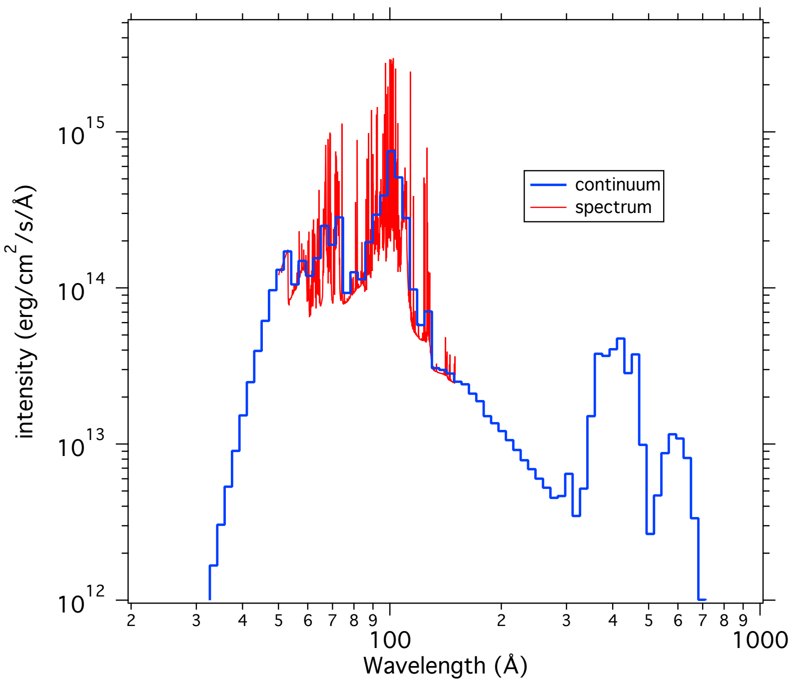


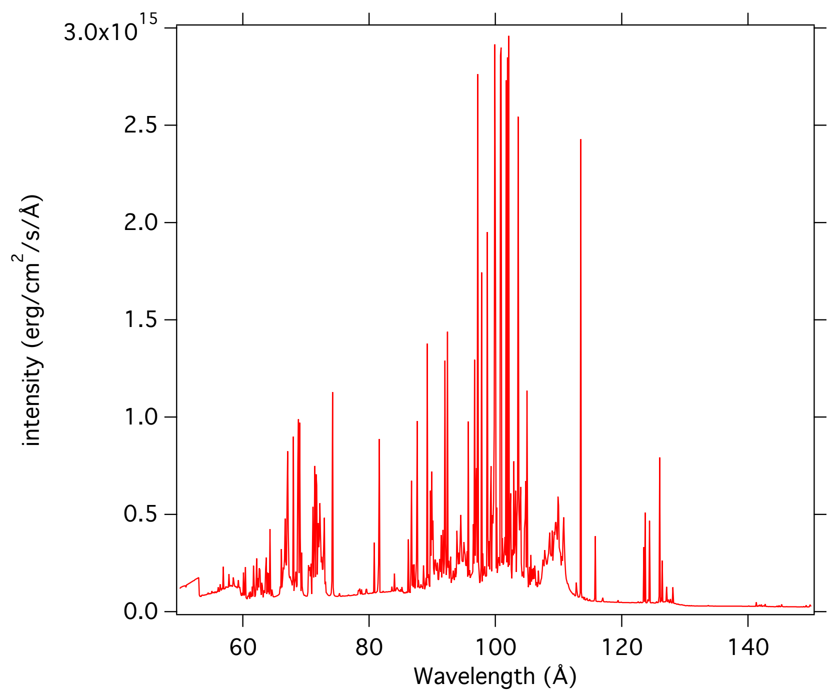
FAC provides detailed data for "K-shell" features

Something more relevant to EUV generation

- Kr plasma sphere
  - R = 1mm
  - T_e = 20 eV, $N_i = 10^{18}$ cm^{-3}
  - FAC atomic model







Summary

Cretin

- combines NLTE atomic kinetics with radiation transport in 1-, 2-, and 3-dimensional geometries
- functions stand-alone or as a postprocessor for rad-hydro codes
- provides compact atomic models suitable for many (non-spectroscopic) applications
- can use atomic models from a variety of sources

Applications include ICF, MFE, laser-produced plasmas, FEL experiments (LCLS, Flash), astrophysics

and EUV generation?